



## DPREP-CHEM

Users Guide for version 5.0.1

March 2018

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## 1. Introduction:

DPREP-CHEM is a tool used to include chemical species to initial and atmospheric boundary conditions in the format required by the model. It depends on an input file named dprep.inp , which must be set according to the domain, simulation data and input file types. This guide aims to present the process of installing and running.

## 2. Structure:

DPREP-CHEM is organized in the follow structure:

- a) bin – Input configuration files and binary file.
- b) bin/build – Configuration files related to the tool compilation.
- c) src - Fortran90 source code.

## 3. Installation and configuration instructions:

a) PHASE I – Environment and compilation.

**DPREP-CHEM compilation is only compatible to PGI and Intel compilers. The gfortran version will be available in the future.**

The examples below are considering a build with Intel compiler.

Download the SPACK in Downloads page \_  
<http://brams.cptec.inpe.br/downloads>.

Unzip the source code file on your desktop , eg /dados/fontes:

```
→ cd /dados/fontes  
→ tar zxvf SPACK-4.3.tar.gz
```

Download DPREP-CHEM-5.0.1.tar.gz from Downloads page  
<http://brams.cptec.inpe.br/downloads>.

Copy zipped file DPREP-CHEM-5.0.1.tar.gz to your working local folder.

```
→ cd /dados/fontes  
→ cp /download/DPREP-CHEM-5.0.1.tar.gz ./
```

Unzip it:

```
→ tar zxvf DPREP-CHEM-5.0.1.tar.gz
```

Create an symbolic link to the desired chemical mechanism, eg “RELACS”:

```
→ cd ./src
```

```
→ ln -fs /dados/fontes/SPACK-4.3/Mechanism/RELACS
```

The DPREP -CHEM also needs the GRIB API installation. Please refer to the site <https://software.ecmwf.int/wiki/display/GRIB/GRIB+API+CMake+installation> For more information about the installation.

Download GRIB API from:

<https://software.ecmwf.int/wiki/display/GRIB/Releases>

Choose a folder to copy the GRIB API:

```
→ mkdir -p /dados/source/
```

Unzip the GRIB API file in that folder:

```
→ cd /dados/source/
```

```
→ tar -xzvf grib_api-1.14.7-Source.tar.gz
```

Create a folder to install the GRIB API:

```
→ mkdir -p /dados/libs/grib_api-1.14.7-intel
```

Create a temporary folder to the build of the GRIB API:

```
→ mkdir -p /dados/libs/build-intel
```

Execute the cmake command inside the build folder, pointing to the source code and the and GRIB API installation folder.

Before running cmake, check whether the libopenjpeg-dev library is already installed. If not, install it:

```
→ apt-get install libopenjpeg-dev
```

Execute the following cmake command:

```
→ cd /dados/libs/build-intel
```

```
→ CC=icc FC=ifort cmake /dados/source/grib_api-1.14.7-Source  
-DCMAKE_INSTALL_PREFIX=/dados/libs/grib_api-1.14.7-intel  
-DENABLE_FORTRAN=ON -DENABLE_JPG=ON -DBUILD_SHARED_LIBS=ON
```

Check if the command result has enabled the features like the example:

```
-- The following features have been enabled:
```

```
* FORTRAN , build the GRIB_API Fortran interface
```

```
* JPG , support for JPG decoding/encoding
```

Make it. If you prefer more than one compiler, use the -j option (-j <number of processors>):

→ `make -j8`

Install it. If you prefer more than one compiler, use the -j option (-j <number of processors>):

→ `make install -j8`

If for any reason there are errors in cmake , compilation or installation, remove all files from the build and installation folder before retrace the steps.

Edit the configuration file ( file `include.mk.intel` for intel ):

→ `gedit /dados/fontes/DPREP-CHEM-5.0.1/Bin/build/include.mk.intel`

Change the path of the GRIB API installation folder and the compiler folder ( intel ) . See Appendix A :

```
FC = /opt/Intel/Bin/ifort
```

```
GRIBLIB=-L/dados/libs/grib_api-1.14.7-intel/lib -lgrib_api_f90 -lgrib_api
```

```
GRIBINC=-I/dados/libs/grib_api-1.14.7-intel/include
```

```
FLOADER = /opt/Intel/Bin/ifort
```

Edit `paths.mk` file, which points to the chemical variables used in BRAMS:

→ `gedit /dados/fontes/DPREP-CHEM-5.0.1/bin/build/paths.mk`

Change the value of the following variable, pointing it to the root BRAMS folder:

```
# USER RELATED
```

```
RAMS_ROOT=/dados/fontes/BRAMS-5.2
```

Compile the code. The `OPT=intel` option includes the `include.mk.intel` file during the make command, and the `CHEM` option selects the chemistry used in BRAMS :

→ `cd /dados/cursos/fontes/DPREP-CHEM-5.0.1/bin/build`

→ `make OPT=intel CHEM=RELACS_TUV`

## b) PHASE II – Execution

Before you start the application you must configure your input options :

→ `gedit /dados/cursos/fontes/DPREP-CHEM-5.0.1/bin/dprep.inp`

Change the following variables. Please refer to the Appendix B.

```

$ARGS_INPUT

!!!! DATE !!!!

init_year = 2016,
init_month = 04,
init_day = 11,
init_hour = 12,

!!!! TIME STEP !!!!!

step = 6,
times = 4,

!!!! ATMOS !!!!!

atmos_type = 0,
atmos_prefix = 'dp',
atmos_sufix = '00',
atmos_idir = './dp/',

!!!! CHEM !!!!!

!10 shadoz, 11 binary clim, 12 oper mocage

chem_type = 11,
chem_merge = .TRUE.,
chem_interp = 1,
chem_ppbmconv = .TRUE.,
chem_idir = './climatology/',

!!!! OUTPUT !!!!!

out_type = 1,
out_prefix = 'dp-chem-relacs-',
out_sufix = '00',
out_dir = './',

$END,

```

Execute the DPREP binary:

```
→ cd ./DPREP-CHEM-5.0.1/bin/
```

```
→ ./dprep_RELACS.x
```

At the end of the run it can be seen that the result consist of files for evaluation ( ctl and gra ) and files that will be used for model input ( vfm ).

Input files:

- Boundary and initial condition atmospheric files:

Boundary and initial condition atmospheric files are converted files from Global GFS to the required format for DPREP-CHEM. The conversion of files is done by GeraDP program, which is also available in BRAMS site, in the Input Data / Atmospheric section.

- Chemical files:

It contains chemical species to be included in the initial conditions and atmospheric boundary in the specific format for the template.

The files are available in BRAMS site , at Input Data / Chemical section.

## Appendix A

Variables	Description and comments
USEHDF4 (deprecated)	enable/disable HDF4 lybrary. 0 = disabled. (default) 1 = enabled .
USEGRIB	Enables/disables the GRIB library . 0 = disabled. 1 = enabled. (default)
GRIBLIB	Path and libraries of GRIB-API. Eg: /usr/lib/grib_api -lgrib_api_f90 – lgrib_api
GRIBINC	Include path of GRIB-API. Eg: /usr/lib/grib_api/include
USENETCDF (deprecated)	Enables/disables the NETCDF library. 0 = disabled. (default) 1 = enabled.
USEPARALLEL	Enables/disables the parallelism 0 = disabled. (default) 1 = enabled.
FC	Compiler for the Fortran source code. Ex: /usr/in/ifort
FC_OPTS	Fortran compilation flags. *Caution* some flags are strictly needed for the well working.
FLOADER	Compiler for linking the objects Eg: /usr/in/ifort

Table 1: Variables for configuration and compilation

## Appendix B

Variables	Description and comments
init_year	Start year Integer type
init_month	Start Month Integer type
init_day	Start day Integer type
init_hour	Start hour Integer type
Step	Time step in hour for conditions to be processed. Ex: 6
Times	Amount of conditions to be generated. Integer type
atmos_type	Atmospheric input file type 0 = DP asc default CPTec.
atmos_prefix	Atmospheric input file prefix Eg='dp'
atmos_sufix	Atmospheric input file suffix. Eg='00'
atmos_idir	Atmospheric input file folder
chem_type	Chemical input file type 10 = vertical profile 11 = binary climatology 12 = operacional mocage.
chem_merge (obsoleto)	Controls whether the files should be concatenated. .true. or .false.
chem_interp	Interpolation type for chemical data. 1 = bilinear.
chem_ppbmconv	Convert the output in ppbm. .true. or .false.
chem_idir	Folder of the chemical files.
out_type	Output file type 1 = vfm
out_prefix	Output file type prefix. Eg = dp-chem-cb07
out_sufix	Output file type suffix. Eg = 00
out_dir	Output folder Ex = .

Table 2: Variables for the configuration and execution.